

X-ray Diffraction Study on LiMoS_2 Intercalation Compound

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Introduction: Metal dichalcogenides, in particular MoS_2 , are known to possess a unique combination of valuable properties, which make them useful as solid lubricants and catalysts for hydrodesulfurization. The material is hexagonal and may be considered as build of Mo-S trigonal prisms stacked along the c axis of the unit cell. The strong covalent bonding between Mo and S and the weak Van-der-Waals interaction between the layers renders the material a good host for intercalation chemistry. For example, species with Li intercalated between Mo-S layers are formed easily. Although several experiments have been carried out the structure of stoichiometric LiMoS_2 is not determined yet with the main difficulty coming from the fact that LiMoS_2 is quite a disordered material.

Methods and Materials: MoS_2 and LiMoS_2 have been subjected to powder x-ray diffraction experiments to determine the structure of the latter. The experiments were carried out with the use of x-rays of energy 30 keV at room temperature.

Results: Experimental structure factors, being the powder diffraction spectra normalized in electron units, are shown in Figure 1. That one of MoS_2 consists of well-defined Bragg peaks - a characteristic typically seen with well-crystallized materials. The corresponding atomic distribution function (PDF), shown in Figure 2, is also composed of well defined peaks. In particular, the first two peaks correspond to Mo-S and Mo-Mo atomic pairs. The structure factor for LiMoS_2 contains a few broad peaks and a pronounced diffuse component. Such a diffraction pattern is typically seen with heavily disordered materials and it is very difficult to be tackled by ordinary techniques for structure determination such as the Rietveld method. The corresponding atomic pair distribution function is rich in structure-related features and lends itself to structure determination. In particular, it is immediately seen that both MoS_2 and LiMoS_2 have similar Mo-S and Mo-Mo coordination. Possible structure models of LiMoS_2 are being explored by fitting them to the experimental atomic distribution function. The results will be reported elsewhere.

Conclusions: The method of atomic pair distribution function is a useful technique for accessing the structure of materials with intrinsic disorder.

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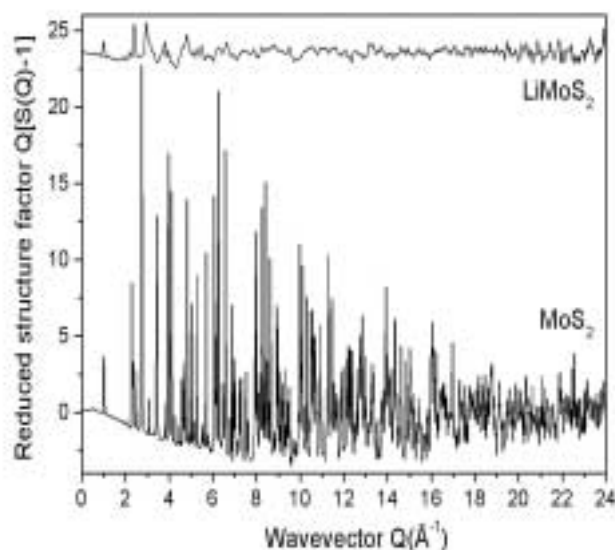


Figure 1. Experimental structure factors for MoS_2 and LiMoS_2 .

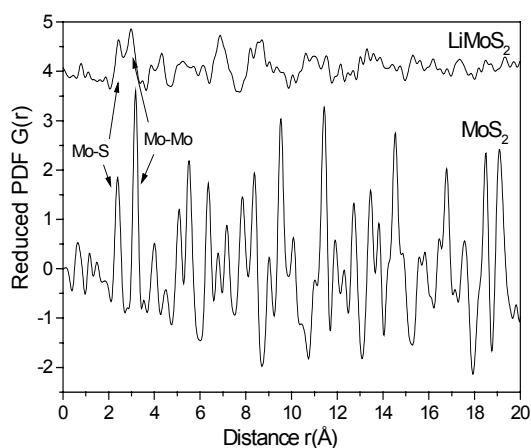


Figure 2. Experimental atomic pair distribution functions for MoS_2 and LiMoS_2 obtained by Fourier transforming the structure factors of Fig. 1.